# A Search for Patterns and Connections

## Highlights of Teller's Contributions to Computational and Mathematical Physics

*January 15, 2008, marks the 100th anniversary of Edward Teller's birth. This highlight is the second in a series of 10 honoring his life and contributions to science.*

EDWARD Teller began thinking about numbers before he was even five years old. In *Memoirs*, he recalls a game he played as he went to sleep. "I knew that a minute has sixty seconds, and I charged myself to discover how many seconds there were in an hour, a day, or a year." For the rest of his life, he continued to look for mathematical patterns in the physical world around him. And many of his insights led to important methods underlying complex calculations used to model physical processes today.

Teller's career in basic science research coincided with the discovery of quantum mechanics, the mathematical theory that provides a framework for studying atomistic behavior. Quantum mechanics can be used to precisely describe phenomena that classical Newtonian physics cannot account for, such as the stability of matter and the microscopic rules governing the physics of atoms. The discovery of quantum mechanics allowed researchers to precisely connect material behavior at the visible (macroscopic) level with that at the invisible level of atoms, molecules, and their constituents. Quantum mechanical ideas, including much of Teller's best work, thus offer potential new methods to compute the detailed properties of matter.

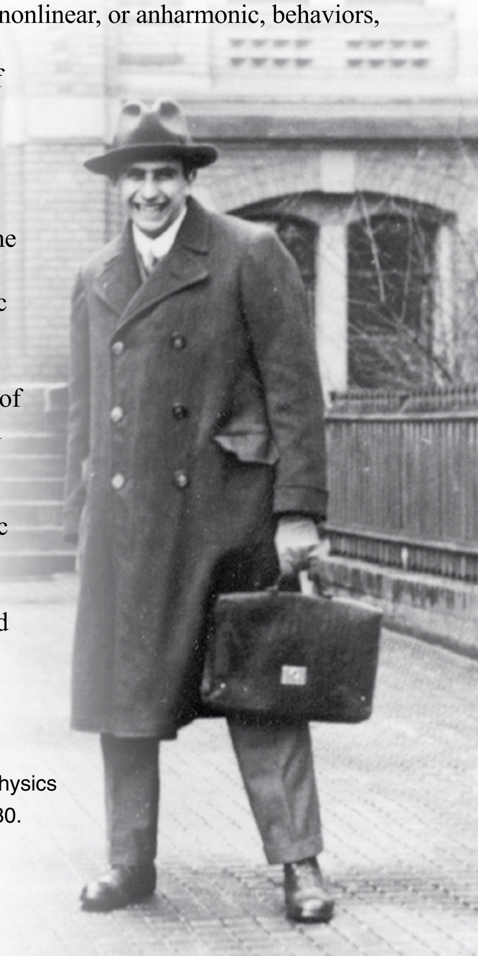
The Metropolis algorithm, which is essential for making statistical mechanics calculations computationally feasible, is perhaps Teller's best-known work in computational physics. (See *S&TR*, January/February 2007, p. 6.) Metropolis resulted from a collaborative effort involving Teller, his former student Marshall Rosenbluth, their wives Mici Teller and Arianna Rosenbluth, and Nicolas Metropolis, who published the algorithm in 1953. Today, it forms a basic part of the arsenal of every computational physicist. Teller was contributing ideas to important statistical mechanics calculations long before his work on Metropolis.

### Quantifying Nonlinear Oscillation

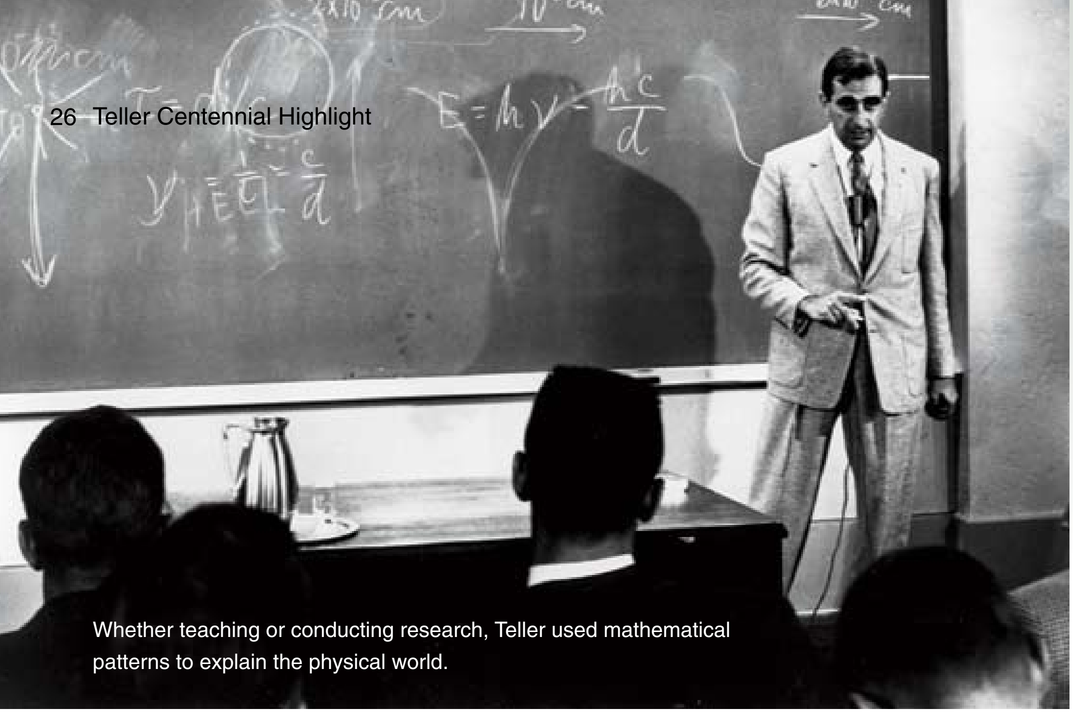
In 1928, Teller transferred from Karlsruhe Technical Institute to the University of Leipzig to study with Werner Heisenberg, a major contributor to the development of quantum mechanics. After receiving a Ph.D. in physics in 1930, he began working at the University of Göttingen, where he applied quantum mechanics to various systems.

Among Teller's many contributions from that time was his work on anharmonic oscillation. A widely applied quantum mechanics calculation describes the dynamics of the harmonic oscillator. Classically, a familiar example is a wire spring, in which the compression or extension is exactly proportional to the force applied. The basic quantum mechanics calculation of this behavior accounts for many of the physical processes occurring in matter, including how the molecular structure of material responds to compression, sound, and heat. However, a harmonic oscillator fails to capture other phenomena such as the expansion that occurs when metal is heated. To model these nonlinear, or anharmonic, behaviors, researchers needed methods to illuminate in detail the effects of the forces between atoms.

At Göttingen, Teller worked with G. Pöschl to study anharmonic oscillators. Their eight-page paper, published in the German journal *Zeitschrift für Physik*, described an anharmonic oscillator that not only could be mathematically solved but also illustrated the detailed behavior of more realistic oscillators. Pöschl and Teller's clever solution was initially thought to be a useful textbook example of anharmonic behavior. Researchers later found it to rely on underlying symmetries that could be applied to physical phenomena from scattering to nonlinear optics.



Edward Teller received a Ph.D. in physics from the University of Leipzig in 1930.



Whether teaching or conducting research, Teller used mathematical patterns to explain the physical world.

## An Exact Solution for a Phase Transition

Teller was also interested in the thermodynamics and statistical mechanics of phase transitions, such as the changes occurring in the structure of water when ice melts. In 1925, Ernst Ising developed a mathematical model for studying a similar phase transition in the spins of ferromagnetic materials. These materials will retain an amount of magnetization up to a specific temperature, at which point the magnetism disappears.

Ising was only able to solve his model for spins in one dimension and thus could not illustrate the mechanics of a phase transition. Many physicists then worked at solving the Ising model in two dimensions. Lars Onsager, who won the Nobel Prize in Chemistry in 1968, succeeded in demonstrating a magnetic phase transition by taking advantage of specific symmetries of the model.

Building on the work of Ising and Onsager, Teller suggested that his student Julius Ashkin generalize Ising's model so it would capture more of the physics occurring in ice phases while preserving the symmetries exploited by Onsager's calculations. The two-dimensional Ashkin–Teller model indeed provided an exact solution for a phase transition such as water freezing, and Ashkin's work on this problem became part of his doctoral thesis. For some time, the Ashkin–Teller model was seen as a clever but niche calculation in statistical physics. In the 1960s, scientists began to discover that the Ising and Ashkin–Teller models were examples of a more general class of theories that provide deeper insights to the thermodynamics of phase transitions. More recently, researchers have found that this general class of models is relevant to string theory.

## A Limited Approximation

Teller's curiosity also led him to search for a simple understanding of the stability of matter. The rigorous approach for modeling the behavior of atoms, molecules, and condensed matter is the Schrödinger equation, which describes the complete quantum dynamics of electrons and nuclei in matter. This equation involves complex calculations that often do not easily reveal the physics involved. Even with today's supercomputers, only relatively simple systems can be analyzed using the full equation.

Instead, for most problems, computational scientists use approximate methods to examine atomistic behavior. Approximations eliminate unimportant elements of a problem so that, ideally, only the essential features remain, thus reducing computational time and increasing physical understanding. In 1955, J. W. Sheldon published a paper on the widely used Thomas–Fermi approximation that intrigued Teller. Sheldon's analysis indicated that, at this level of approximation to the full Schrödinger equation, the nitrogen molecule would be unstable. Teller wondered if Sheldon's results indicated a general limitation of the Thomas–Fermi approximation. In a concise paper written in honor of his friend Eugene Wigner and published in 1962 in *Reviews of Modern Physics*, Teller showed that the Thomas–Fermi approximation insufficiently captured the physics expressed in the more complex Schrödinger equation. Later, mathematical physicists such as Elliott Lieb used Teller's arguments in explaining how the Schrödinger equation produced stable matter.

## The Quest Continues

Throughout his life, Teller sought simple but incisive explanations to better understand the structure of matter. As these examples show, many discoveries borne out of this quest led to unexpected findings that often had practical applications. One of Teller's many legacies to Lawrence Livermore is the simultaneous pursuit of basic science to understand the physical world and applied science to use that knowledge.

*—Carolin Middleton*

**Key Words:** anharmonic oscillator, Ashkin–Teller model, computational physics, Edward Teller, mathematical physics, Metropolis algorithm, Schrödinger equation, Thomas–Fermi model.

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